Visualizing paired electron pockets in the underdoped cuprates using ARPES in the presence of current

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(Dated: September 25, 2012)

We propose an experiment to test a theory of the underdoped cuprates, which assumes that the pseudogap contains a phase-incoherent paired electron pocket and unpaired hole pockets. The proposed experiment involves angular-resolved photoemission spectroscopy (ARPES) measurements performed in the pseudogap regime and in the presence of a transport current running through the sample. The current leads to two main effects on the spectral function: First, even a weak current tilts the Fermi surface and is predicted to open up a part of the electron pocket if the energy of the incident photons is smaller but close to the pseudogap. Second, stronger currents suppress pairing of the electron pocket, which too can be observable by ARPES. The observation of these predicted phenomena, including their temperature and current dependencies, should clarify the central question about the existence of pairs in the enigmatic pseudogap region.

PACS numbers: 74.72.-h, 74.72.Kf, 79.60.-i, 74.25.Sv

The effort to understand the behavior of copper oxide superconductors [1] has lasted for decades. Theoretically, there are a large number of competing explanations [2] for the cuprates. They have been studied from the strongly correlated side at low doping or from weakly interacting models from the overdoped side of the phase diagram [3–14]. Despite serious efforts by theorists to explain the nature of the pseudogap, a consensus has not been reached and many key issues remain open. Among them is the question about the nature of the excitations in the pseudogap and in particular whether there exist preformed electronic pairs above the superconducting transition.

In this paper we propose and model an experiment that would help clarify this question and in particular may help to unambiguously determine whether the enigmatic pseudogap region contains “ghost” electron pockets. Specifically, we propose to perform angular-resolved photoemission spectroscopy (ARPES) measurements in the presence of a current, which should produce useful data visualizing excitations that may otherwise be hidden due to pairing or gaps associated with other competing orders.

While the usefulness of this proposed experiment is not limited to a particular theoretical model, we focus on the specific model of paired electron pockets [15, 16], which we believe is strongly supported by three recent experimental developments. First, recent work has observed a proximity-induced pseudogap [17] and supports the idea that the pseudogap is connected to paired quasiparticles. Second, the experimental discovery [18–20] of small Fermi pockets in the pseudogap phase of underdoped cuprates motivates a description which incorporates Fermi surface reconstruction. The apparent discrepancy between full Fermi pockets and the “Fermi arcs” observed by ARPES can be resolved with a model [21] consistent with what we consider here [16]. Third, there is a nodal-anti-nodal dichotomy observed in STM [22] and Raman [23] experiments. This is where nodal excitations have an energy which decreases with decreasing doping, and anti-nodal excitations have a larger energy which increases with decreasing doping.

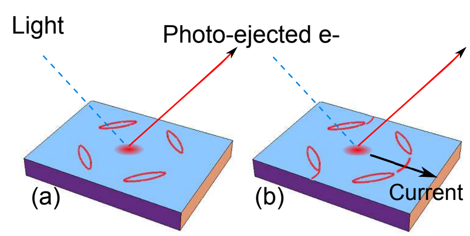

FIG. 1. (color online) A qualitative illustration of the experimental setup and the predicted phenomenon: (a) the incident light and ejected electrons that initially leave the electron pockets hidden due to a pairing gap; (b) the electron-pockets are partially revealed in the ARPES signal due to a current running through the sample along the anti-nodal direction. The incident photon energy and direction of the current can be controlled to reveal hidden pairing.

These key ingredients, pairing, Fermi surface reconstruction, and the nodal-anti-nodal dichotomy, are incorporated in a recent theoretical proposal describing the pseudogap phase of underdoped cuprates [16]. In this theory, the pseudogap is attributed to strongly-paired (but uncondensed) electron pockets in the anti-nodal region, mediated by orientational spin fluctuations (that suppress long-range Néel order in an initially antiferromagnetic metal) and unpaired hole-pockets in the nodal regions (with a weak tendency for p-wave pairing; the hole pairing is assumed to be destroyed by temperature in the pseudogap). This is shown to be equivalent to d-wave pairing when the Brillouin zone is unfolded [15, 16, 24]. Note that in the paired electron pocket scenario the key players are “ghost” electrons, which are always hidden from direct visualization due to a large pairing gap. Clearly, the main objective of an experiment that intends to test this picture is to unbind the electrons without destroying the underlying Fermi surface.

This situation might have been achieved in the quantum oscillation experiments, where the large applied field effectively acts as a BCS upper critical field opening up the Fermi surface and yielding oscillations. However, ARPES measurements cannot be done in such a large field. Other possibilities include suppressing pairing by temperature and/or disorder, however they alone cannot reveal the “ghost” Fermi surface and will just smear it out.

To test if the pseudogap is made of paired but uncondensed electronic excitations we propose an ARPES experiment in the presence of a current as shown in Fig. 1. There are two central reasons for applying a current. As we show, even a weak current will reveal the paired bands by shifting the spectrum. For larger currents complete depairing can occur opening up the “ghost” Fermi surface that should be visible by ARPES. This is pragmatic when the gap has already been reduced by raising the temperature so that the depairing current has a magnitude practical for experiment.

Setup and model: We consider a hole-doped cuprate superconductor in the pseudogap regime subjected to a uniform current $\boldsymbol{J}$ as shown in Fig. 1(b). Our main goal is to determine key qualitative features of an ARPES spectrum measured in the presence of the current. We adopt a simplified model, which is consistent with the theory developed in Ref. 16 and contains the essential ingredients to reliably calculate the key features of the ARPES spectrum predicted by the theory. According to this theory the pseudogap phase emerges from a strongly fluctuating critical antiferromagnetic state with reconstructed Fermi-surfaces consisting of electron-like pockets in the anti-nodal regions $(\pi/a, 0)$ and $(0, \pi/a)$ and hole-like pockets in the nodal regions $(\pm\pi/2a, \pm\pi/2a)$. The key formal ingredient is to describe the components of the *physical* electron in a rotated reference frame set by the local spin-density wave (SDW) order $\boldsymbol{\varphi} = z^*_\sigma \boldsymbol{\sigma}_{\sigma\sigma'} z_{\sigma'}$, where the bosonic spinon field z_σ defines the SU(2) rotation. This parametrization of the physical electron gives rise to an emergent gauge field, which plays a crucial role in the pairing of the fermions. The pseudogap phase is characterized by strongly s-wave paired (but uncondensed) electron pockets and hole pockets [25] that remain unpaired (a weak p-wave pairing in the hole pockets is assumed to be suppressed by temperature). Here, we adopt a simple minimal model for the pseudogap phase which nevertheless captures the key features necessary to address an ARPES experiment in the presence of current:

$$H = \sum_{\boldsymbol{k}} \sum_{\alpha=\pm} \left[\xi_{\boldsymbol{k}f} f^\dagger_{\boldsymbol{k}\alpha} f_{\boldsymbol{k}\alpha} + \xi_{\boldsymbol{k}h} h^\dagger_{\boldsymbol{k}\alpha} h_{\boldsymbol{k}\alpha}\right] - \sum_{\boldsymbol{k}} \left[\Delta f^\dagger_{\boldsymbol{k}+} f^\dagger_{-\boldsymbol{k}-} + h.c.\right] + \frac{\Delta^2}{\lambda}, \quad (1)$$

where $f_{\boldsymbol{k}\pm}$ and $h_{\boldsymbol{k}\pm}$ are the annihilation operators for the electron-like and hole-like excitations with momentum $\boldsymbol{k}$, respectively, and $\pm$ labels the charge associated with the emergent gauge field. The sum over $\boldsymbol{k}$ is performed over the reduced Brillouin zone. We note that $f_{\boldsymbol{k}\alpha}$ becomes the physical electron in the SDW ordered state, where the spinon field z_σ condenses and the $\pm$ indices become equivalent to the electron spin indices. Pairing in the electron pockets is included at the mean-field level by introducing a real s-wave pair potential Δ. The spectra are given by $\xi_{\boldsymbol{k}f,h} = (\xi_{\boldsymbol{k}} + \xi_{\boldsymbol{k}+\boldsymbol{Q}})/2 \pm [(\xi_{\boldsymbol{k}} - \xi_{\boldsymbol{k}+\boldsymbol{Q}})^2 + 4\varphi^2]^{1/2}/2$, where $\xi_{\boldsymbol{k}} = -2t(\cos k_x a + \cos k_y a) - 4t' \cos k_x a \cos k_y a - \mu$. Here, $\boldsymbol{Q} = (\pi/a, \pi/a)$, and we will take $t' = -0.3t$ and $\mu = -0.6t$ [26]. The quantity φ is the uniform SDW order parameter, but we stress that φ is used here merely to parameterize the underlying Brillouin zone folding, and that in reality, spin fluctuations are expected to suppress long-range antiferromagnetic order in the pseudogap phase. In the above, $\lambda > 0$ is the effective attractive interaction for the electrons generated by the gauge fluctuations. Since the pseudogap phase is not characterized by long-range SDW order the attractive interaction mediated by the gauge fluctuations is, in principle, long-ranged [16].

We emphasize here that a calculation of the current within model (1) would give rise to a phase-coherent superflow, which is not correct. In the pseudogap, pairs have formed but transport is in terms of holes and phase-incoherent pairs of charge $2e$. However, the excitation spectrum in the presence of current should be correctly obtained from these expressions and can reliably calculate the spectral function, which is the central quantity of interest.

Spectral function for a current-carrying pseudogap: We now study modifications to the ARPES spectrum when a current is applied to a cuprate superconductor in the pseudogap regime. Although ARPES is a probe of the physical electron spectral function we will compute the spectral functions for the electron- and hole-like excitations in this work. In the presence of spinon fluctuations we cannot, in principle, expect the physical electronic spectrum to be identical to that of the electron-like excitations [21]. However, as we will show, the application of even a weak current can cause sections of the electron pockets to appear or disappear. Furthermore, a strong enough current will completely depair the electron pockets and reveal their entire Fermi surfaces. Despite our simplified treatment, these key modifications should persist also in the ARPES spectrum as well.

The current endows the Cooper pairs with a center-of-mass momentum $\boldsymbol{q}_{\boldsymbol{J}}$, and the single-particle Green function in the presence of a uniform current can be written as [27, 28]

$$\check{G}_{\boldsymbol{k}}(i\omega_n) = \left[\hbar(i\omega_n - \boldsymbol{v}_{\boldsymbol{k}} \cdot \boldsymbol{q}_{\boldsymbol{J}})\check{1} - \xi_{\boldsymbol{k}f}\check{\tau}_3 + \Delta\check{\tau}_1\right]^{-1}, \quad (2)$$

where $\omega_n = (2n+1)\pi k_B T$ are the fermionic Matsubara frequencies, $\boldsymbol{v}_{\boldsymbol{k}} = \partial\xi_{\boldsymbol{k}f}/\hbar\partial\boldsymbol{k}$, checks indicate matrices in Nambu space, and $\check{\tau}_i$ are the Pauli matrices. The gap is then obtained from the following self-consistent condition,

$$1 = \frac{\lambda}{N} \sum_{\boldsymbol{k}} \frac{1 - n_F(E^+_{\boldsymbol{k}}) - n_F(E^-_{\boldsymbol{k}})}{2E_{\boldsymbol{k}}}, \quad (3)$$

where n_F is the Fermi-Dirac distribution function and $E^\pm_{\boldsymbol{k}} = E_{\boldsymbol{k}} \pm \hbar\boldsymbol{v}_{\boldsymbol{k}} \cdot \boldsymbol{q}_{\boldsymbol{J}} = [\xi^2_{\boldsymbol{k}f} + \Delta^2]^{1/2} \pm \hbar\boldsymbol{v}_{\boldsymbol{k}} \cdot \boldsymbol{q}_{\boldsymbol{J}}$. The retarded Green function for the + electrons, $G^R_{\boldsymbol{k}+}(\omega)$, then defines the corresponding spectral function $A_{\boldsymbol{k}+}(\omega) = -\mathrm{Im}G^R_{\boldsymbol{k}+}(\omega)/\pi$. One then

finds,

$$A_{\boldsymbol{k}+}(\omega) = s_{\boldsymbol{k}}^2\delta(\hbar\omega - \xi_{\boldsymbol{k}h}) + r_{\boldsymbol{k}}^2\left[u_{\boldsymbol{k}}^2\delta(\hbar\omega - E_{\boldsymbol{k}}^+) + v_{\boldsymbol{k}}^2\delta(\hbar\omega + E_{\boldsymbol{k}}^-)\right], \quad (4)$$

where $r_{\boldsymbol{k}}^2 = [1 + (\xi_{\boldsymbol{k}} - \xi_{\boldsymbol{k+Q}})/(\xi_{\boldsymbol{k}f} - \xi_{\boldsymbol{k}h})]/2$ and $s_{\boldsymbol{k}}^2 = [1 - (\xi_{\boldsymbol{k}} - \xi_{\boldsymbol{k+Q}})/(\xi_{\boldsymbol{k}f} - \xi_{\boldsymbol{k}h})]/2$, and the Bogoliubov coherence factors are given by $u_{\boldsymbol{k}}^2 = (1 + \xi_{\boldsymbol{k}f}^2/E_{\boldsymbol{k}})/2$ and $v_{\boldsymbol{k}}^2 = (1 - \xi_{\boldsymbol{k}f}^2/E_{\boldsymbol{k}})/2$. Although, interaction and disorder effects beyond the scope of our simplified model will inevitably give rise to non-trivial self-energy corrections and modifications to (4), we are eventually interested in looking at the robust equal-energy contours of the dispersions rather than the level widths, which are sensitive to a self-energy. Therefore, (4) should correctly convey the main qualitative effects of the applied current on the spectral function.

Depairing due to current: The gap solution to (3) as a function of $\boldsymbol{q_J}$ along the anti-nodal direction is shown in Fig. 2. As illustrated in the inset, the gap is plotted for the spectrum $\xi_{\boldsymbol{k}f}$ in (a) and, for comparison, for the regular parabolic spectrum $\xi_{\boldsymbol{k}}^0 = \hbar^2k^2/2m - \mu$ in two dimensions in (b). The gap is normalized by Δ_0, which is its value at zero temperature and zero current. The values $\varphi = 0.3t$ and $t/\lambda = 0.7$ were used in (a), and $N_0\lambda \approx 0.34$, where N_0 is the density of states at the Fermi level, was used in (b).

We find that the Fermi velocity for the electron pockets is $\hbar v_F/a \approx 1.3t$. The depairing scale should then be set by $q_J^c \sim \Delta_0/\hbar v_F$. As we see in Fig. 2(a), at zero temperature, the gap remains robust up to this scale and then shows a steep but gradual decrease. A general rounding of the features is observed at finite temperatures. For the parabolic dispersion at $T = 0$, the gap remains robust for $\hbar v_F q_J < \Delta_0$, then sharply drops to zero at the critical depairing scale $\hbar v_F q_J^c \sim \Delta_0$. At finite temperatures, the gap monotonically and smoothly goes to zero. We note that the shoulder for the $T = 0$ result in Fig. 2(a) appears because the gap equation (3) sums the doppler shift over a non-trivial Fermi surface corresponding to the dispersion $\xi_{\boldsymbol{k}f}$. The depairing scale Δ_0 is set by the pseudogap scale, and can be reduced by raising the temperature of the sample until $\Delta_0(T)$ is sufficiently small. Here, $\Delta_0(T)$ is the gap at temperature T and zero current. To the best of our knowledge, depairing effects in two-dimensional conventional superconductors have not been thoroughly investigated, since the initial interest in the early days of BCS theory was in three-dimensional materials. Many investigations of three dimensional *s*-wave [29–31], two dimensional *d*-wave [32, 33] and other exotic pairing [34, 35], however, have been done.

For a weak current, one can obtain an approximate analytic expression for the gap. Solving (3) perturbatively, one finds that the gap as a function of current (in the anti-nodal direction) is given by:

$$\Delta(q_J) \approx \Delta_0(T)\left[1 - \gamma(\hbar v_F q_J/\Delta_0)^2\right], \quad (5)$$

$$\gamma = \left(\frac{ta\Delta_0}{\hbar v_F \Delta_0(T)}\right)^2 \frac{\sum_{\boldsymbol{k}} \frac{\tanh x_{\boldsymbol{k}}\,\mathrm{sech}^2 x_{\boldsymbol{k}}}{4E_{\boldsymbol{k}}^0}\left(\frac{\hbar v_{x\boldsymbol{k}}}{k_B T a}\right)^2}{\sum_{\boldsymbol{k}}\left[\frac{\tanh x_{\boldsymbol{k}}}{(E_{\boldsymbol{k}}^0)^3} - \frac{\mathrm{sech}^2 x_{\boldsymbol{k}}}{2T(E_{\boldsymbol{k}}^0)^2}\right]},$$

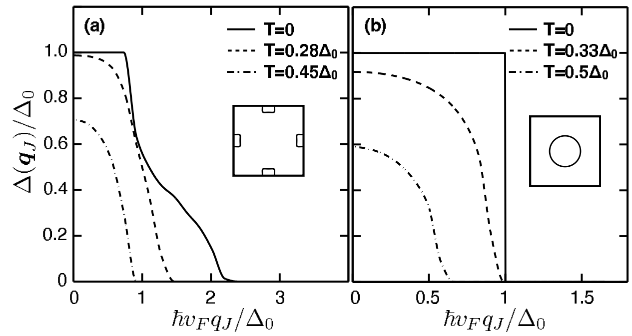

FIG. 2. Solution to the gap equation (3) as a function of q_J along the anti-nodal direction. In (a), the solution is obtained for electrons with spectrum $\xi_{\boldsymbol{k}f}$ (with the Fermi surface shown in the inset), while in (b) we consider the regular isotropic spectrum $\xi_{\boldsymbol{k}}^0 = \hbar^2k^2/2m{-}\mu$ (with the circular Fermi surface as shown in the inset). The gap is normalized with respect to its value at zero temperature and zero current.

with $x_{\boldsymbol{k}} = E_{\boldsymbol{k}}^0/2T$ and $E_{\boldsymbol{k}}^0 = [\xi_{\boldsymbol{k}f}^2 + \Delta_0^2(T)]^{1/2}$. For the $T = 0.45\Delta_0$ result in Fig. 2(a), we find $\Delta_0(T = 0.45\Delta_0) \approx 0.71\Delta_0$. In this case, $\gamma \approx 0.58$, and the perturbative treatment here describes the initial downturn in the gap.

Spectral function results: From (4) we see that the spectral function is non-zero when either (i) $\hbar\omega - \hbar\boldsymbol{v_k}\cdot\boldsymbol{q_J} - E_{\boldsymbol{k}} = 0$ or (ii) $\hbar\omega - \hbar\boldsymbol{v_k}\cdot\boldsymbol{q_J} + E_{\boldsymbol{k}} = 0$. We see that the effect of the Doppler shift is to move the energy scale $\hbar\omega$ away or towards the quasiparticle bands $\pm E_{\boldsymbol{k}}$ depending on the sign of $\hbar\boldsymbol{v_k}\cdot\boldsymbol{q_J}$. While the depairing current scale set by $q_J^c \sim \Delta_0/\hbar v_F$ can require a large current, all that is required here is to use a small $\hbar\boldsymbol{v_k}\cdot\boldsymbol{q_J}$ to just cross into either of the $\pm E_{\boldsymbol{k}}$ bands. In Fig. 3, we plot the spectral function (4) at photon energies just below [Fig. 3(a)] and above [Fig. 3(b)] the upper paired band for zero and finite current. We consider the case where the current is applied in the anti-nodal direction, and also in the nodal direction [Fig. 3(c)]. Plotted on the left are a cut of the paired band dispersion along the $k_y = 0$ line in the Brillouin zone (indicated by the red dashed line on the right in (a)), and the photon energies are indicated by the dotted lines. In (a), the photon energy is set inside the gap at zero current and hence the electron pockets are initially not observed. However, once the current is applied, the paired spectrum at $\boldsymbol{k}$ points where $\boldsymbol{v_k}$ is parallel to $\boldsymbol{q_J}$ is shifted up in energy while the spectrum at $\boldsymbol{k}$ points where $\boldsymbol{v_k}$ is anti-parallel to $\boldsymbol{q_J}$ is shifted down in energy. This leads to the appearance of some sections of the electron pockets. In Figs. 3(b),(c) the photon energy crosses both the hole and the upper paired bands. The application of the current here leads to the disappearance of some sections of the electron pockets.

We remind the reader that the spectral functions plotted in Fig. 3 (see (4)) are for the electron-*like* excitations residing in the anti-nodal regions of the Brillouin zone (we are ignoring the hole-like spectral function here). For the ARPES spectrum, the spectral function must be computed in the physical electron basis obtained from rotating back our electron-like excitations using the spinon field z_σ. In the absence of

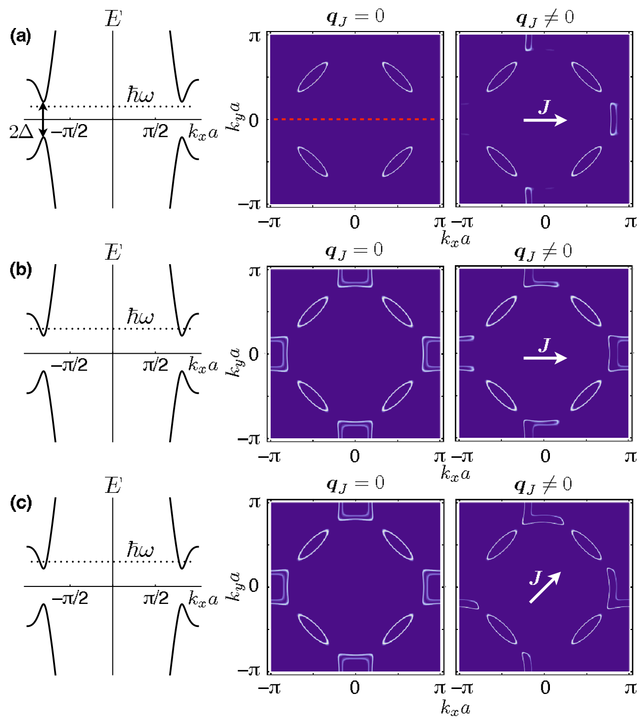

FIG. 3. (color online) Spectral function at zero and finite current for photon energy $\hbar\omega$ just below [see (a)] and above $E_{\boldsymbol{k}}$ [see (b)]. As indicated by the white arrows, the current is applied along the antinodal direction in (a) and (b), and the nodal direction in (c). Paired bands on the left are plotted along the $k_y = 0$ line in the Brillouin zone, as indicated by the red dashed line. In principle, an arbitrarily small q_J can reveal or erase parts of the electron pockets as long as the photon energy is tuned close to the edge of a paired band (see text for details).

long-range Néel order, these spinons are uncondensed and the spinon fluctuations are known to play an important role in the ARPES spectrum [21]. Nevertheless, the appearance and disappearance of the electron-like Fermi surfaces found in this work should have a clear signature in the ARPES spectrum as well. This is because to lowest order the physical electron spectral function is simply a convolution of the spectral functions of its composite electron-like and spinon particles [21]. The appearance or disappearance of the Fermi surface for the fermion component should then directly affect the convolved spectral function.

Heuristically, we now provide the relationship between the drift momentum $\boldsymbol{q_J}$ and the current density based on the Drude model. The total current $\boldsymbol{J} = \boldsymbol{J}_b + \boldsymbol{J}_h$ is composed of holes from the hole pockets $\boldsymbol{J}_h = \sigma_h \boldsymbol{E} = (n_h e^2 \tau_h/m_h)\boldsymbol{E}$ and from uncondensed pairs $\boldsymbol{J}_b = \sigma_b \boldsymbol{E} = (n_b(2e)^2\tau_b/2m_e)\boldsymbol{E}$. Here, n_b is the number density of uncondensed pairs and n_h is the density in the hole pockets. In the pseudogap phase we have a mix of two dissipative fluids whose conductivities will add $\boldsymbol{J} = (\sigma_b + \sigma_h)\boldsymbol{E}$. At steady state, $\boldsymbol{q_J} = 2e\boldsymbol{E}\tau_b$. This means that for a given $\boldsymbol{J}$ the drift momentum is related to total current via $\boldsymbol{q_J} = 2e\boldsymbol{J}\tau_b/(\sigma_b + \sigma_h)$.

The simplest estimate for the critical depairing current density is $J_c = 2en\Delta_0/mv_F$, where n is the density of charge carriers. Specific tight-binding models for $Bi_2Sr_2CaCu_2O_8$ (BSCCO) can be taken from Refs. 26 and 36. In BSCCO, $v_F \approx 250$km/s [37], and the effective mass is ≈ 3-$4m_e$ [38]. A typical carrier density in BSCCO [39] is $n \approx 10^{21}\text{cm}^{-3}$. Therefore, $J_c \approx 65\Delta_0\text{A/cm}^2$ for Δ_0 in units of Kelvin. The energy scale for Δ_0 can be estimated as follows. The ARPES pseudogap can be identified by two energy scales [40], with a low-energy scale given by the location of the leading-edge midpoint and a higher-energy one by the position of a broad peak. The broad maximum of the ARPES spectra are between 100-200meV [41] and the leading-edge midpoint are between around 20-30meV [40]. Scanning tunneling spectroscopy [42] in BSCCO also sees a pseudogap feature around 70-90meV. Ref. 22 also sees a high energy feature in their data in the 60-100meV range. In Ref. 16, the pairing scale is identified as $\Delta_0 \approx 200$K consistent with the low energy features in ARPES and the downturn in uniform spin susceptibility occurs around 300-400K. The observation of a proximity induced pseudogap [17] sees a feature in the normal density of states at around sample bias 10meV. This would correspond to a gap smaller than the low energy feature, but due to gap attenuation in the proximity effect, this might be consistent with the small pseudogap scale. Using $\Delta_0 \approx 200$K, one finds $J_c \approx 1.3 \times 10^4$ A/cm^2. The magnitude of this estimate is not unreasonable if we note that a bulk critical current density of 2-5$\times 10^6$ A/cm^2 has been obtained for BSCCO [43, 44].

In conclusion, we have shown that the application of a weak current during ARPES in the pseudogap state provides a test of the model proposed in Ref. 16, by either revealing sections of the electron pockets, or causing them to disappear, depending on the incident photon energy and current direction. We have also solved the two dimensional gap equation in the presence of a current, establishing the critical depairing current scale $\hbar v_F q_J^c = \Delta_0$ for a circular Fermi surface but depends on Fermi surface geometry in general (Fig. 2). To pragmatically reach the depairing current, Δ_0 needs to be reduced by, for instance, temperature. While the photo-ejected electron's trajectory will be modified by the presence of a weak field induced by the current, it can be accounted for. We have thereby provided a falsifiable test for a model of the cuprate pseudogap.

Acknowledgments: G. R. B. and S. T. would like to thank B. M. Fregoso and Ribhu Kaul for discussions. This research was supported by DOE-BES DESC0001911 (S. T. and V. G.).

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